FUN3D v12.7 Training

Session 4: Gridding, Solution, and Visualization Basics

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Learning Goals

What we will cover

- Basic gridding requirements and formats
- · Nondimensionalizations and axis conventions
- · Basic environment for running FUN3D
- FUN3D user inputs
- Running FUN3D for typical steady-state RANS cases
 - Compressible transonic turbulent flow over a wing-body using a tetrahedral VGRID mesh
 - Turbulent flow over a NACA 0012 airfoil section
- Things to help diagnose problems
- Visualization overview

What we will not cover

- · Other speed regimes
- Unsteady flows



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Gridding Considerations

- FUN3D is a node-based discretization
 - To get similar resolution when comparing with a cell-centered code, you must use a finer grid
 - E.g., on a tetrahedral grid, the grid for FUN3D must be ~2 times finer on the surface, and ~6 times finer in the volume mesh to be fair
 - This is critical when comparing with cell-centered solvers
 - Hanging nodes are not currently supported
- FUN3D integrates all of the way to the wall for turbulent flows
 - Wall function grids are not adequate
 - Goal is to place first grid point at y+=1
 - Base \(\Delta \) on a flat plate estimate using your Reynolds number; can examine result in solver output and tweak as necessary
- Users employ all of the common grid generators VGRID, AFLR2/AFLR3/SolidMesh, ICEM, Pointwise, etc.
- FUN3D also supports point-matched, multiblock structured grids through Plot3D file input
 - Subject to certain grid topologies:
 - Singularities treated i.e., hexes with collapsed faces converted to prisms
- But hexes with 180° internal angles cause FUN3D discretization to break down (LSQ)
- FUN3D can convert tetrahedral VGRID meshes to mixed elements
- FUN3D can convert any mixed element grid into tetrahedra using command line option `--make_tets'



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Supported Grid Formats

Grid Format	Formatted	Unformatted	Supports mixed elements	Direct load or converter	File extension(s)
FAST	х	х		Direct	.fgrid, .mapbc
VGRID (single or multisegment)		х		Direct	.cogsg, .bc, .mapbc
AFLR3	Х	X Also Binary	х	Direct	.ugrid/.(I)r8.ugrid/.(I)b8.ugrid, .mapbc
FUN2D	х			Direct	.faces
Fieldview v2.4, v2.5, v3.0	х	х	х	Direct (Some details of format not supported)	.fvgrid_fmt, .fvgrid_unf, .mapbc
Felisa	х			Direct	.gri, .fro, .bco
Point-matched, multiblock Plot3D	Х	Х	Hexes, degenerates	Converter	.p3d, .nmf
CGNS		Binary	Х	Converter	.cgns

The development team can work with you to handle other formats as needed



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Boundary Condition Input File

Where required, the FUN3D .mapbc file takes the form:

```
Number of boundary patches
Boundary patch index BC index Family name
```

- The BC index may be either a 4-digit FUN3D-style index or a GridTool-style index
- The family name is optional, but must be present if the user requests patch lumping by family

```
3
1 4000 Wing
2 5000 Farfield
3 6662 Symmetry plane
```

 Exception: The .mapbc format for VGRID meshes follows the GridTool/VGRID format



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Nondimensionalization

- Notation: * indicates a dimensional variable, otherwise dimensionless; the reference flow state is usually free stream ("∞"), but need not be
- Define reference values:

 $-L_{ref}^*$ = reference length of the physical problem (e.g. chord in ft)

 $-L_{ref}$ = corresponding length in your grid (dimensionless)

 $-\rho_{ref}^*$ = reference density (e.g. slug/ft³)

 $-\mu_{ref}^{r}$ = reference molecular viscosity (e.g. slug/ft-s)

 $-T_{ref}^*$ = reference temperature (e.g. °R, compressible only)

 $-a_{ref}^*$ = reference sound speed (e.g. ft/s, compressible only)

 $-U_{ref}^*$ = reference velocity (e.g. ft/s)

• Space and time are made dimensionless in FUN3D by:



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Nondimensionalization (cont)

For the compressible flow equations the dimensionless variables are:

$$\begin{split} -\vec{u} &= \vec{u}^* / a_{ref}^* & \text{so } |\vec{u}|_{ref} = |\vec{u}|_{ref}^* / a_{ref}^* = M_{ref} \\ -P &= P^* / (\rho_{ref}^* a_{ref}^{*2}) & \text{so } P_{ref} = P_{ref}^* / (\rho_{ref}^* a_{ref}^{*2}) = 1/\gamma \\ -a &= a^* / a_{ref}^* & \text{so } a_{ref} = 1 \\ -T &= T^* / T_{ref}^* & \text{so } T_{ref} = 1 \\ -e &= e^* / (\rho_{ref}^* a_{ref}^{*2}) & \text{so } e_{ref} = e_{ref}^* / (\rho_{ref}^* a_{ref}^{*2}) = 1/(\gamma(\gamma-1)) + M_{ref}^2 / 2 \\ -\rho &= \rho^* / \rho_{ref}^* & \text{so } \rho_{ref} = 1 \end{split}$$

- From the equation of state and the definition of sound speed:

$$T = \gamma P / \rho = a^2$$

 The input Reynolds number in FUN3D is related to the Reynolds number of the physical problem by

reynolds_number = $\mathrm{Re}_{\mathit{ref}}/L_{\mathit{ref}}$ where $\mathrm{Re}_{\mathit{ref}}=\rho_{\mathit{ref}}^*U_{\mathit{ref}}^*L_{\mathit{ref}}^*/\mu_{\mathit{ref}}^*$ i.e. reynolds_number is a Reynolds number **per unit grid length**



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Setting the Reynolds Number Input

- Frequent cause of confusion, even for developers
- Need to know what characteristic length your Reynolds number is based on – mean aerodynamic chord, diameter, etc.
- Your input Reynolds number is based on the corresponding length of that "feature" in your computational grid
- Example: You want to simulate a Reynolds number of 2.5 million based on the MAC:
 - If the length of the MAC in your grid is 1.0 grid units, you would input Re=2500000 into FUN3D
 - If the length of the MAC in your grid is 141.2 grid units (perhaps these physically correspond to millimeters), you would input 2500000/141.2, or Re=17705.4 into FUN3D

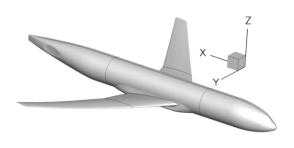


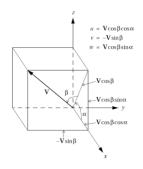
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FUN3D Axis Convention





- FUN3D coordinate system differs from the standard wind coordinate system by a 180° rotation about the y-axis
 - Positive x-axis is toward the "back" of the vehicle (downstream)
 - · Positive y-axis is out the "right wing"
 - · Positive z-axis is "upward"
- · The freestream angle of attack and yaw angle are defined as shown



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Runtime Environment

- "Unlimit" your shell (also good idea to put this in any queue scripts):
 - \$ ulimit unlimited # for bash
 - \$ unlimit # for c shell
- If unformatted or binary, what "endianness" does your grid file have?
 - E.g., VGRID files are always big endian, regardless of platform
 - If your compiler supports it, FUN3D will attempt to open files using an open (convert=...) syntax
 - Most compilers support some means of conversion
 - Either an environment variable or compile-time option, depending on what compiler you're using
 - E.g., Intel compiler can be controlled with an environment variable
 F UFMTENDIAN = big
- Memory required by solver: rough rule of thumb is 3-3.5 GB per million points (not cells!)
 - Conversely, 200k-300k points per 1 GB of memory
 - Users generally partition into smaller domains than this, but be aware of these numbers
 - This memory estimate will be higher if visualization options are used, etc



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User Inputs for FUN3D

Input deck fun3d.nml

- The user is required to supply an input deck for FUN3D named fun3d.nml (fixed name)
- This filename contains a collection of Fortran namelists that control FUN3D execution – all namelist variables have default values as documented
- But user will need to set at least some high-level variables, such as the project name

Command Line Options (CLOs)

- CLOs always take the form --command_line_option after the executable name
 - Some CLOs may require trailing auxiliary data such as integers and/or reals
- · User may specify as many CLOs as desired
- CLOs always trump fun3d.nml inputs
- CLOs available for a given code in the FUN3D suite may be viewed by using
 --help after the executable name
- Most CLOs are for developer use; namelist options are preferred where available



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Transonic Turbulent Flow on a Tetrahedral Wing-Body Mesh



- For this case, we will assume that someone has provided a set of VGRID files containing the mesh
 - f6fx2b_trn.cogsg, f6fx2b_trn.bc, and f6fx2b_trn.mapbc
- It is always a good idea to examine the .mapbc file first to check the boundary conditions and any family names
 - Note that specific boundary conditions will be covered in a separate session



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Transonic Turbulent Flow on a Tetrahedral Wing-Body Mesh

- For this case, the VGRID/GridTool-style .mapbc file is as shown
- Surface grid consists of 51 patches
- Note that VGRID/GridTool-style BC's are specified
- Family names are also as shown (required in this format)
- FUN3D does not use the other columns of data
- If you cannot easily visualize your mesh to set appropriate boundary conditions, one easy approach is to set them all to inflow/outflow, then run a single time step of FUN3D with boundary visualization activated – then set patch BC's as needed for actual simulation



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FUN3D 1

Transonic Turbulent Flow on a Tetrahedral Wing-Body Mesh



 Now we will look at the minimum set of user inputs needed in fun3d.nml to run this case



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Transonic Turbulent Flow on a Tetrahedral Wing-Body Mesh

```
project_rootname = 'f6fx2b_trn'
/
                                                        Project name
         &raw grid
           grid_format = 'vgrid'
                                                        Read a set of VGRID files
         &reference_physical_properties
mach_number = 0.75
                                                       Sets freestream Mach number
            reynolds number = 17705.40
                                                        Sets Reynolds number
            angle_of_attack = 1.0
                                                        Sets freestream angle of attack
           temperature = 580.0
temperature_units = "Rankine"
                                                       Sets freestream temperature
Uses Rankine temperature units for input
         &code_run_control
            restart_read = 'off'
                                                        Perform a cold start
                                                        Perform 500 time steps
            steps
                           = 500
         &force_moment_integ_properties
           area_reference = 72700.0
x_moment_length = 141.2
                                                       Sets reference area
                                                       Sets length for normalizing y-moments
                                                                                                       All in
                                                        Sets length for normalizing x-, z-moments
            y moment length = 585.6
                                                                                                     grid units
            x_moment_center = 157.9
                                                        Sets x-moment center
            z_moment_center = -33.92
                                                       Sets z-moment center
         &nonlinear_solver_parameters
                                                        CFL for meanflow is ramped from 10.0 to 200.0
            schedule_cfl
            schedule_cflturb = 1.0 30.0
                                                        CFL for turbulence is ramped from 1.0 to 30.0
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                                                                                              FUN3D
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```

Transonic Turbulent Flow on a Tetrahedral Wing-Body Mesh

- We now have the boundary conditions and input deck set up to run FUN3D
- To execute FUN3D, we use the following basic command line syntax:

```
mpirun ./nodet_mpi
```

- Note your environment may require slightly different syntax:
 - mpirun **VS** mpiexec **VS** aprun **VS** ...
 - · May need to specify various MPI runtime options:
 - -np #
 - -machinefile filename
 - -nolocal
 - · Others



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Transonic Turbulent Flow on a Tetrahedral Wing-Body Mesh

- Using 1 Intel Haswell node (24 cores), this case runs in 2-3 minutes
- The top of the screen output will include an echo of your fun3d.nml, as well as some preprocessing information:

Transonic Turbulent Flow on a Tetrahedral Wing-Body Mesh

- · At this point, time stepping commences
- · For each time step:
 - The L2-norm of the density turbulence equation is red|blue; max and location are also included
 - Lift and drag are reported in green
- · "Done." indicates execution is complete

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Transonic Turbulent Flow on a **Tetrahedral Wing-Body Mesh**

- At this point, time stepping commences
- For each time step:
 - The L2-norm of the density|turbulence equation is red|blue; max and location are also included
 - Lift and drag are reported in green
- "Done." indicates execution is complete

```
er density_RMS density_MAX X-location Y-location Z-location turb_RMS turb_MAX X-location Y-location Z-location 1 0.56745420002834ZE+00 0.28035E+02 0.16377E+03 -0.1656ZE+03 0.2017E+02 0.764159584901741E+04 0.13249E+07 0.79654E+04 -0.88280F±04 0.26767E+1
         Lift 0.103222129717669E+00
                                                                  Drag 0.646514468368827E+00
         0.300676687726037E+00 0.12718E+02 0.29226E+03 -0.72487E+02 -0.12411E+02 0.753354469872627E+04 0.12868E+07 0.79654E+04 -0.88280E+04 0.25675E+02
         Lift 0.146830367737086E+00
                                                                  Drag 0.721243419758588E+00
      0.235098406158263E-04 0.44827E-02 0.63496E+04 -0.38199E+04 0.18712E+04 0.799698877237297E-01 0.12961E+02 0.46732E+04 -0.15204E+04 0.26710E+03
               0.556610229549889E+00
                                                                          0.388376897833650E-01
      0.232908407834686E-04 0.44201E-02 0.63496E+04 -0.38199E+04 0.18712E+04 0.789246351974423E-01 0.12785E+02 0.46732E+04 -0.15204E+04 0.26710E+03
       Lift 0.556607946389416E+00
                                                                Drag 0.388374809483346E-01
Writing f6fx2b trn.flow (version 11.8) lmpi io 2
 inserting current history iterations 500
Time for write: .0 s
Done
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                                                                                                                      FUN3D
```

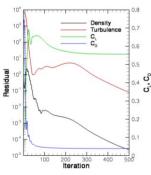
Transonic Turbulent Flow on a Tetrahedral Wing-Body Mesh

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- FUN3D provides a couple of text files with basic statistics and summary data:
 - f6fx2b trn.grid info File containing basic mesh statistics and partitioning info File containing force breakdowns by boundary and totals - f6fx2b trn.forces
- FUN3D also produces:

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f6fx2b trn hist.dat Tecplot file with residual, force convergence histories Solver restart information f6fx2b_trn.flow



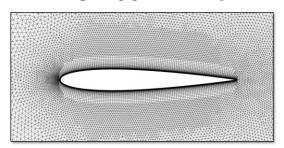
- · For this particular case, the mean flow and turbulence residuals are reduced by ~5 orders of magnitude over 500 time steps
- Lift and drag come in after a few hundred time steps

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FUN3D

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NACA 0012 Airfoil



- For this case, we have been given a set of binary, big endian AFLR3 files
 - 0012.b8.ugrid, 0012.mapbc
 - For computations in 2D mode
 - Grid must be one-element wide in the y-direction (except when using FUN2D format)
 - Grid must contain only prisms and/or hexes
- First check the .mapbc file
 - The y-planes must be separate boundary patches and should be given BC 6662



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0012.mapbc

4

1 4000

2 5000

3 6662

4 6662



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NACA 0012 Airfoil

&global

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boundary_animation_freq = -1

- fun3d.nml is shown here
- FUN2D grid format will automatically be executed in 2D mode; all others must be explicitly put in 2D mode

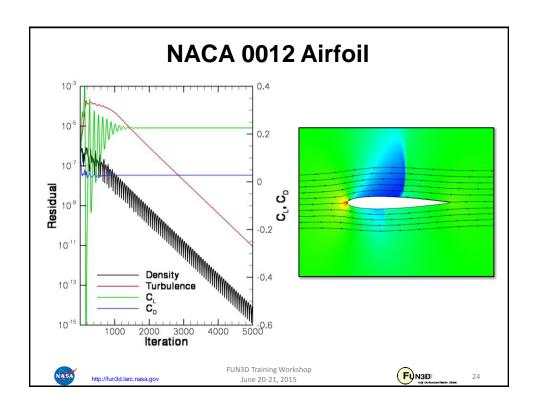
&project project_rootname = '0012' &raw grid Read an AFLR3 grid grid format = 'aflr3' twod_mode = .true. Execute in 2D mode &reference_physical_properties mach_number = 0.80
reynolds_number = 1.e6
angle_of_attack = 1.25 temperature temperature_units = "Rankine" &code run control restart_read = 'off' = 5000 steps &force moment integ properties area reference = 0.1 x_moment_center = 0.25 &nonlinear_solver_parameters schedule cfl = 10.0 200.0 schedule_cflturb = 1.0 10.0



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FUN3D
July Sectoral Medie: Stelen

```
NACA 0012 Airfoil
FUN3D 12.7-74063 Flow started 05/18/2015 at 09:06:46 with 24 processes
 [Echo of fun3d.nml]
The default "stream" data format is being
                                                                                                                                Binary AFLR3 format is the default
used for the grid format "aflr3".
Preparing to read binary AFLR3 grid: 0012.b8.ugrid
                                                                                                                                 Binary AFLR3 grid being read
                                                                                                                                Grid contains 116,862 points
Grid contains 204,510 tris, 14,607 quads
Grid contains 102,255 prisms, 7,047 hexes
   ntface,nqface
  ntet,npyr,nprz,nhex 0 0 102255 7047
cell statistics: type,
cell statistics: prz, 0.16960303E-06, 0.52577508E-01, 164.861624007 cell statistics: hex, 0.83173480E-09, 0.12843645E-04, 123.906431556 cell statistics: all, 0.83173480E-09, 0.52577508E-01, 164.861624007
 ... PM (64, skip_do_min) :
      ... Calling ParMetis (ParMETIS_V3_PartKway) ....
... edgeCut 11490
... Time for ParMetis: .1 s
      ... checking for spanwise edge cuts.
... Constructing partition node sets for level-0...
      ... Edge Partitioning ....
... Boundary partitioning....
... Euler numbers Grid:1 Boundary:0 Interior:0
      ... Reordering for cache efficiency....
... ordering edges for 2D.
... Write global grid information to 0012.grid_info
            Time after preprocess TIME/Mem(MB): 0.31 90.82
  NOTE: kappa_umuscl set by grid: .00
 Grid read complete
 Using 2D Mode (Node-Centered)
                                                                                                                                 Solver running in 2D mode
Distance_function unique ordering T 20000000
construct partial boundary...nloop=
   find closer surface edge...
 Wall spacing: 0.100E-03 min, 0.100E-03 max, 0.100E-03 avg
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```



List of Key Input/Output Files

- Input
 - Grid files (prefixed with project name, suffixes depend on grid format)
 - fun3d.nml
- Output
 - [project].grid info
 - [project].forces
 - [project]_hist.dat
 - [project].flow



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What Could Possibly Go Wrong?

Problem

 Common complaint from VGRID meshes during initial preprocessing phase at front end of solver:

- This is due to a very old VGRID bug that causes an incompatibility between the .cogsg and .bc files
 - Compile and run utils/repair_vgrid_mesh.f90 to generate a valid
 .bc file to replace your original one



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What Could Possibly Go Wrong?

Problem

 Common complaint from unformatted/binary meshes during initial preprocessing phase at front end of solver:

Read/Distribute Grid.

forrtl: severe (67): input statement requires too much data, unit 16100, file /misc/work14/user/FUN3D/project.cogsg

Check the endianness of the grid and your environment/executables

Problem

- Unexpected termination, especially during preprocessing or first time step
 - Are your shell limits set?
 - Do you have enough local memory for what you are trying to run?



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What Could Possibly Go Wrong?

Problem

- Solver diverges or does not converge
 - Problem-dependent, very tough to give general advice here
 - Sometimes require first-order iterations (primarily for high speeds)
 - Sometimes require smaller CFL numbers
 - Sometimes require alternate flowfield initialization (not freestream) in some subregion of the domain: e.g., chamber of an internal jet
 - Check your boundary conditions and gridding strategy
 - Perhaps your problem is simply unsteady

Problem

- Solver suddenly dies during otherwise seemingly healthy run
 - Sometimes useful to visualize solution just before failure
 - Is it a viscous case on a VGRID mesh? Try turning on large_angle_fix in &special_parameters namelist (viscous flux discretization degenerates in sliver cells common to VGRID meshes)
 - Is it a turbulent flow on a mesh generated using AFLR3? Look for "eroded" boundary layer grids near geometric singularities – AFLR3 sometimes has trouble adding viscous layers near complex corners, etc



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What Could Possibly Go Wrong?

In General...

- Do not hesitate to send questions to <u>fun3d-support@lists.nasa.gov</u>;
 we are happy to try to diagnose problems
 - Please send as much information about the problem/inputs/environment that you can, as well as all screen output, any error output, and config.log
 - In extreme cases, we may request your grid and attempt to run a case for you to track down the problem
 - If you cannot send us a case due to restrictions, size, etc, a generic/smaller representative case that behaves similarly can be useful
 - Check the manual for guidance
- Ask the FUN3D user community, fun3d-users@lists.nasa.gov



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Visualization Learning Goals

- · What this will teach you
 - Run-time flow visualization output
 - Output on boundary surfaces
 - Output on user-specified "sampling" surfaces within the volume
 - Output of full volume data
 - Output generated by "slicing" boundary data "sectional" output
- What you will not learn
 - The plethora of output options available for visualization
 - Tecplot usage
- What should you already know
 - Basic flow solver operation and control



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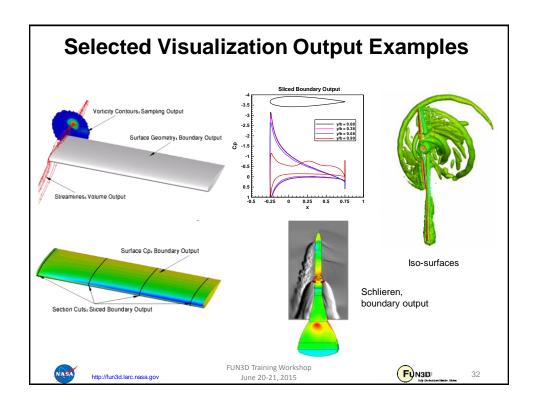
Background

- Datasets are getting simply too large to post-process in a traditional manner
- FUN3D allows visualization data to be generated as the solver is running
 - · User specified frequency and output type
 - User specified output variables from a fairly extensive list
- Majority of output options are Tecplot-based
 - Volume output may also be generated in Fieldview, CGNS formats
- Note FUN3D also supports true in-situ visualization at scale using the DoE VisIt package; however, this is not covered here
 - Intelligent Light is currently integrating Visit's in-situ capabilities with Fieldview



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Visualization Overview

- All of the visualization outputs require similar namelist-specified "frequency" N to activate:
 - In all cases, N = 0, 1, 2, 3, ...
 - N = 0 generates no output
 - N < 0 generates output only at the *end* of the run typically used for steady-state cases. The actual value of N is ignored
 - N > 0 generates output every Nth time step typically used to generate animation for unsteady flows; can also be used to observe how a steady flow converges



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Visualization Overview

- Customizable output variables (except sliced boundary data):
 - Most variables are the same between the boundary surface, sampling and volume output options; boundary surface has a few extra
 - See manual for lists of all available variables
 - Default variables always include x, y, z, and the "primitive" flow variables u, v, w, and p (plus density if compressible)
 - Several "shortcut" variables: e.g., primitive variables = rho, u, v, w, p
 - Must explicitly turn off the default variables if you don't want them
 (e.g. primitive variables = .false.)
 - Variable selection for each co-processing option done with a different namelist to allow "mix and match"



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Visualization Overview

 For boundary surface output, default is all solid boundaries in 3D and one y=const plane in 2D; alternate output boundaries selected with, e.g.:

- If you already have a converged solution and don't want to advance the solution any further, can do a "pass through" run:
 - Set steps = 0 in &code run control
 - You must have a restart file ([project].flow)
 - Run the solver with the appropriate namelist input to get desired output
 - [project].flow will remain unaltered after completion



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Visualization Overview

- Sampling output requires additional data to describe the desired sampling surface(s)
 - Specified in namelist &sampling_parameters
 - Surfaces may be planes, quadrilaterals or circles of arbitrary orientation, or may be spheres or boxes
 - Isosurfaces and schlierens also available
 - Points may also be sampled
 - See manual for complete info
- Sliced boundary surface output requires additional data to describe the desired slice section(s)
 - Specified in namelist &slice data
 - Always / only outputs x, y, z, C_p, C_{fx}, C_{fy}, C_{fz}
 - User specifies which (solid) boundaries to slice, and where
 - See manual for complete info



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Visualization Overview

- Output files will be ASCII unless you have built FUN3D against the Tecplot library (exception: sliced boundary data is always ASCII)
 - ASCII files have .dat extension
 - Binary files have .plt extension smaller files; load into Tecplot faster
 - Boundary output file naming convention (T = time step counter):
 - [project]_tec_boundary_timestepT.dat if N > 0
 - [project]_tec_boundary.dat if N < 0
 - Volume output file naming convention (note: 1 file per processor P)
 - [project]_partP_tec_volume_timestepT.dat if N > 0
 - [project] partP tec volume.dat if N < 0
 - Sampling output file naming convention (one file per sampling geometry G):
 - [project] tec sampling geomG timestepT.dat if N > 0
 - [project]_tec_sampling_geomG.dat if N < 0



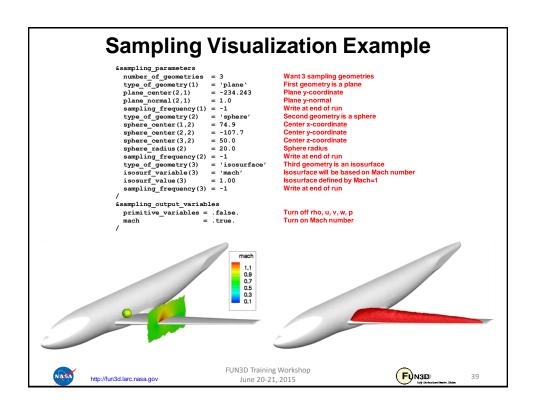
http://fun3d.larc.nasa.gov

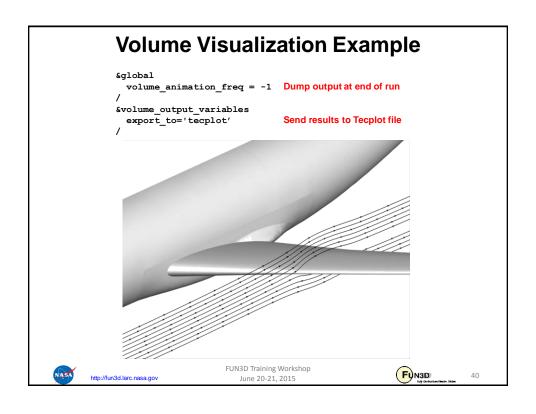
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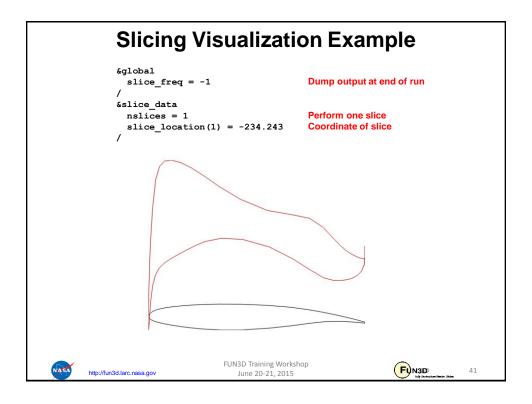


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Boundary Output Visualization Example &global boundary_animation_freq = -1 / &boundary_output_variables primitive_variables = .false. cp = .true. yplus = .true. Turn off rho, u, v, w, p Turn on Cp Turn on y / FUN3D Training Workshop June 20-21, 2015







Troubleshooting/FAQ

- I can see what look like ragged dark lines on sampling surfaces and volume data – what is that?
 - Duplicate information at partition boundaries is not removed; if surface is not completely opaque, double plotting locally doubles the opaqueness (duplicate info *is* removed from boundary surface output)
 - Turn off transparency in Tecplot
- When I dump out volume plot files in Tecplot format, I get a file for every processor – is there a way around this?
 - Not currently. However, Tecplot can be easily told to load all of the files at once without having to individually select them all.
 - The team is working with Tecplot to develop their next generation of I/O API's, with special focus on massively parallel needs
 - Alternative: switch to Fieldview or CGNS output, which uses a single file



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What We Learned

- · Basic gridding requirements and file formats
- · Runtime environment
- How to set up boundary conditions and very basic FUN3D input decks
- How to run a tetrahedral RANS solution for a wing-body VGRID mesh
- How to perform a 2D mixed element airfoil solution using an AFLR3 grid
- · Some unhealthy things to watch for and possible remedies
- · Overview of visualization output options and examples

Don't hesitate to send questions our way! fun3d-support@lists.nasa.gov



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